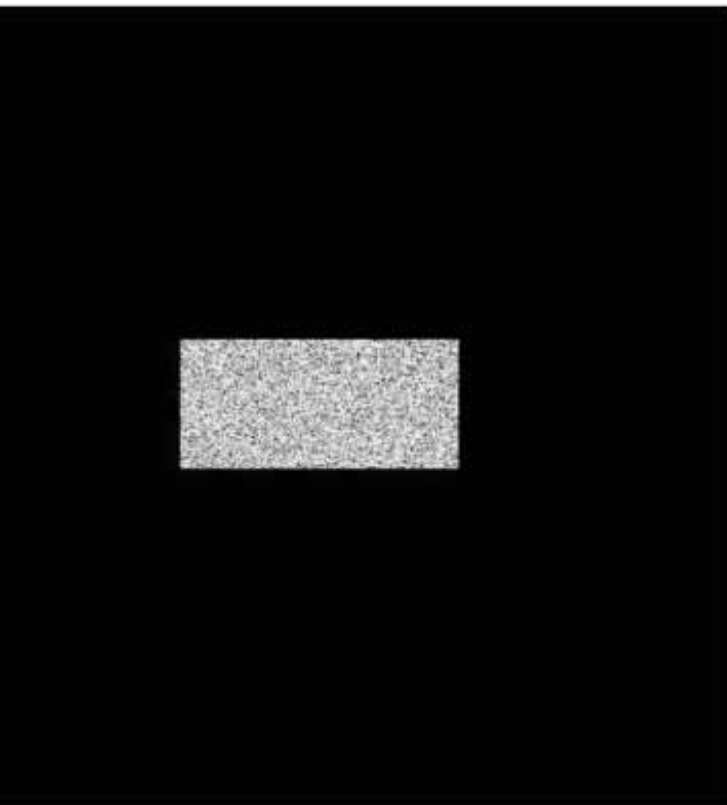




getting the most  
from your elect

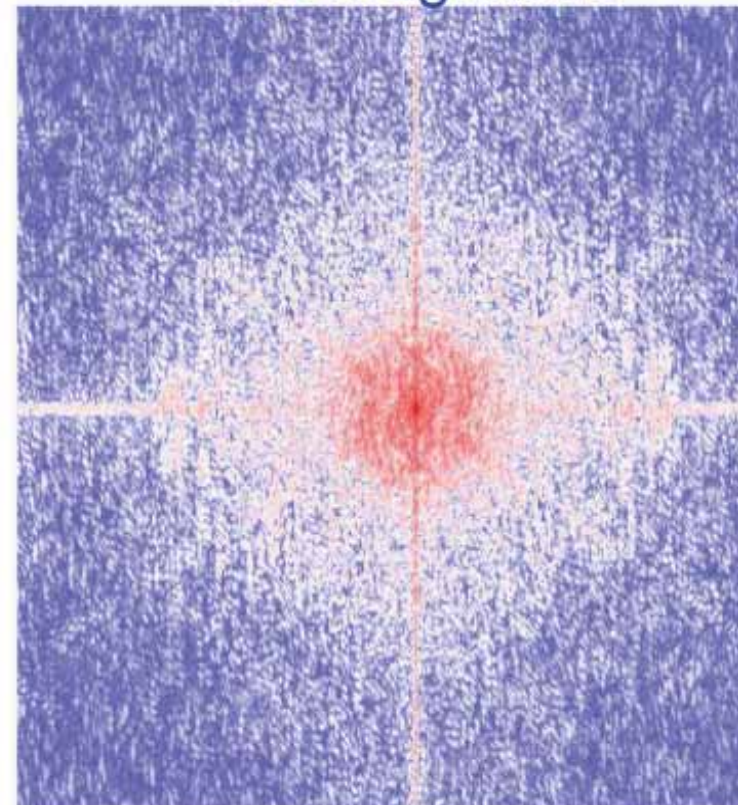
Garth W  
6 June 2

start with a random guess



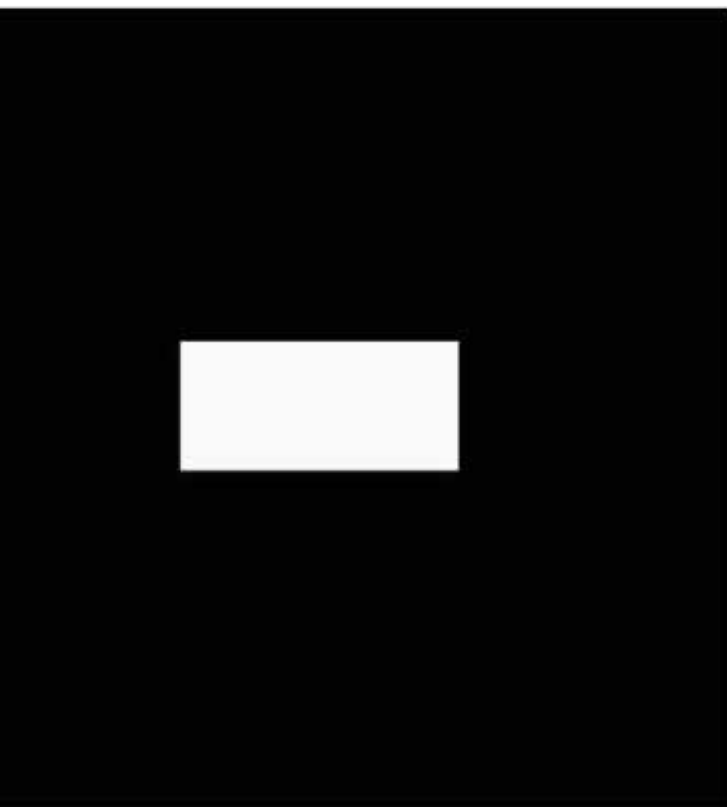
enforce the object support

Measured intensity replaces  
the magnitude



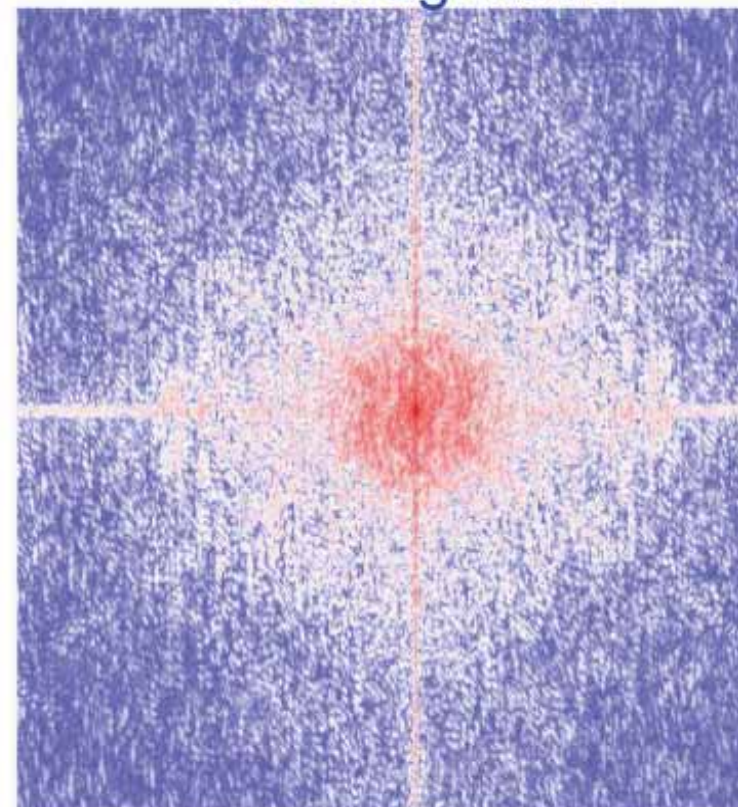
*but keep the calculated phase*

Propagate constrained wave



enforce the object support

Measured intensity replaces  
the magnitude



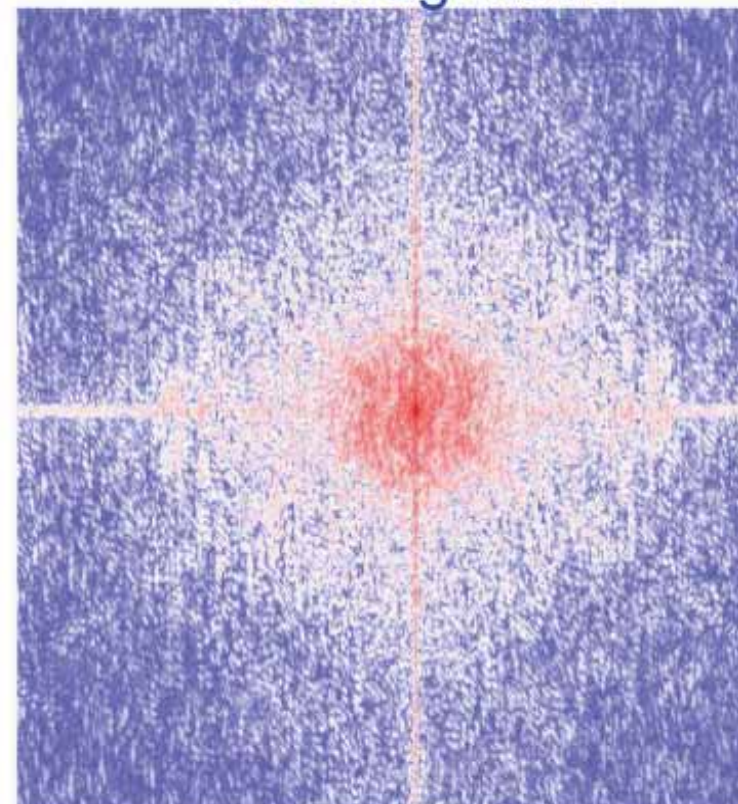
*but keep the calculated phase*

Stop when converged



enforce the object support

Measured intensity replaces  
the magnitude



*but keep the calculated phase*

## retrieval algorithms: a comparison

APPLIED OPTICS/Vol. 21/2758/1982

Iterative algorithms for phase retrieval from intensity data are compared to gradient search methods. Both the problem of phase retrieval from two intensity measurements (in electron microscopy or wave front sensing) and the problem of phase retrieval from a single intensity measurement plus a non-negativity constraint (in astronomy) are considered, with emphasis on the latter. It is shown that both the error-reduction algorithm for the problem of a single intensity measurement and the Gerchberg-Saxton algorithm for the problem of two intensity measurements converge. The error-reduction algorithm is also shown to be closely related to the steepest-descent method. Other algorithms, including the input-output algorithm and the conjugate-gradient method, are shown to converge in practice much faster than the error-reduction algorithm.

Soc. Am. A/Vol. 4, No. 1/January 1987

J. R. Fienup

Rev. Sci. Instrum. **78**, 011301 (2007); doi:10.1063/1.2403783 (10 pages)

## Invited Article: A unified evaluation of iterated projection algorithms for phase retrieval

**S. Marchesini**

*Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, California 94550-9234  
Biophotonics Science and Technology, University of California, Davis, 2700 Stockton Boulevard  
Sacramento, California 95817*

## retrieval by iterated projections

20, Issue 1, pp. 40-55 (2003)

doi:10.1364/JOSAA.20.000040

# Extending the methodology of X-ray crystallography to allow imaging of micrometre-sized non-crystalline specimens

Jianwei Miao\*, Pambos Charalambous†, Janos Kirz\*  
& David Sayre\*‡

\* *Department of Physics and Astronomy, State University of New York  
Stony Brook, New York 11794-3800, USA*

† *Kings College, Strand, London WC2R 2LS, UK*



# High-resolution *ab initio* three-dimensional x-ray diffraction microscopy

Henry N. Chapman, Anton Barty, Stefano Marchesini, Aleksandr Noy, and Stefan P. Hau-Riege

University of California, Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, California 94550

Congwu Cui, Malcolm R. Howells, and Rachel Rosen

Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720

Haifeng He, John C. H. Spence, and Uwe Weierstall

Department of Physics and Astronomy, Arizona State University, Tempe, Arizona 85287-1504

Tobias Beetz, Chris Jacobsen, and David Shapiro

Department of Physics and Astronomy

Received August 26, 2005; revised October 14,

Coherent x-ray diffraction microscopy is limited, in principle, by only the wavelength fraction imaging with high resolution in  $z$  reconstructed volume images. These images are *a priori* knowledge about the shape or content of a nonperiodic object. We also construct two-dimensional projections of the reconstructed volume images. We also construct two-dimensional projections of the reconstructed volume images. We also construct two-dimensional projections of the reconstructed volume images.

OCIS codes: 340.7460, 110.1650, 110.6

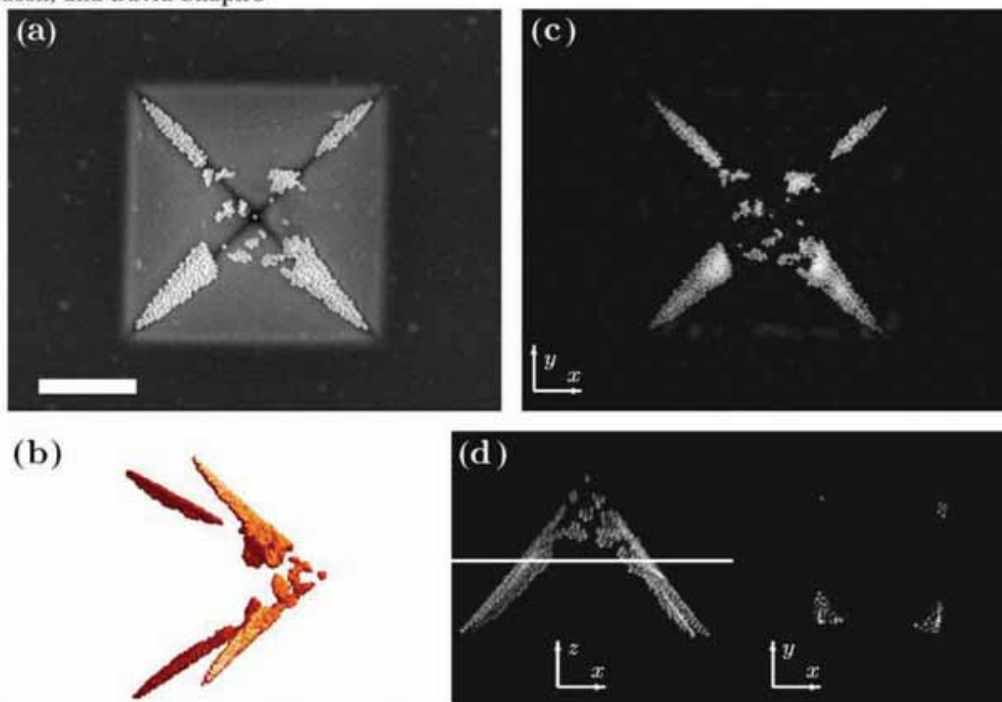


Fig. 2. (Color online) (a) SEM image of the pyramid test object, consisting of 50-nm-diameter gold spheres lining the inside of a pyramid-shaped indentation in a 100-nm-thick silicon nitride membrane. The membrane extends over a window of size  $50\ \mu\text{m} \times 1.7\ \text{mm}$ , the pyramid base width is  $2.5\ \mu\text{m}$ , and the height is  $1.8\ \mu\text{m}$ . (b) Isosurface rendering of the reconstructed 3D image. (c) Extremely large depth-of-field x-ray projection image from a central section of the 3D diffraction data set, reconstructed with the Shrink-wrap algorithm. (d) Maximum value projection of the 3D reconstructed image (left) with a horizontal white line indicating the location of a tomographic slice (right). The scale-bar length is  $1\ \mu\text{m}$  and applies to all images.

## LETTERS

## Three-dimensional mapping of a deformation field inside a nanocrystal

Mark A. Pfeifer<sup>1</sup>†, Garth J. Williams<sup>1</sup>†, Ivan A. Vartanyants<sup>1</sup>†, Ross Harder<sup>1</sup> & Ian K. Robinson<sup>1</sup>†

PHYSICAL REVIEW B **76**, 115425 (2007)

### Orientation variation of surface strain

R. Harder,<sup>1</sup> M. A. Pfeifer,<sup>2</sup> G. J. Williams,<sup>3</sup> I. A. Vartanyants,<sup>4</sup> and I. K. Robinson<sup>1</sup>

<sup>1</sup>London Center for Nanotechnology, Department of Physics and Astronomy, University College, London WC1E 6L

<sup>2</sup>Department of Physics, La Trobe University, Victoria 3086, Australia

<sup>3</sup>School of Physics, University of Melbourne, Victoria 3010, Australia

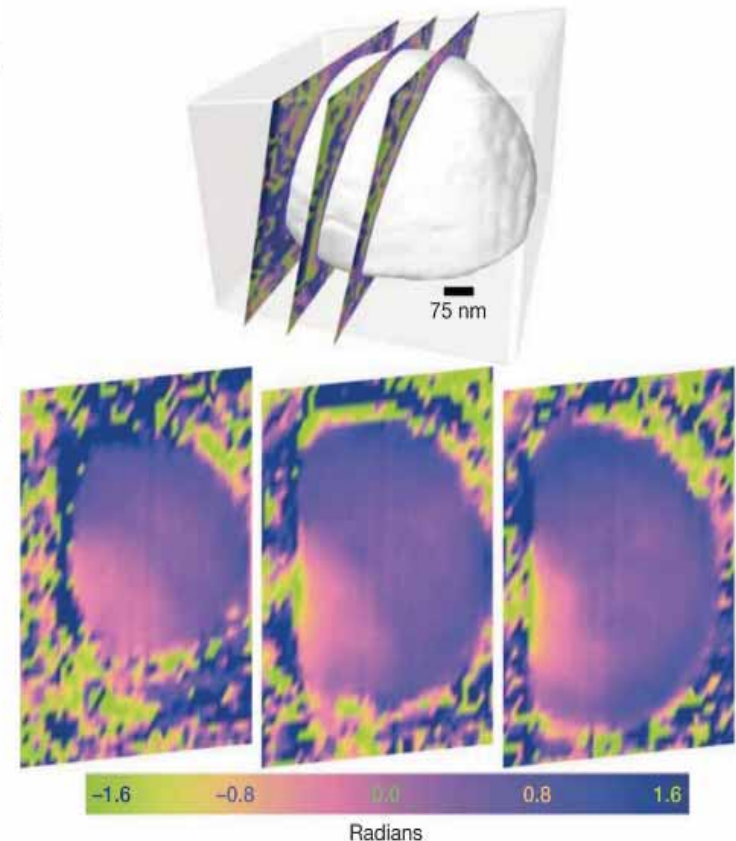
<sup>4</sup>HASYLAB, DESY, Notkestrasse 85, D-22607 Hamburg, Germany

(Received 2 July 2007; published 20 September 2007)

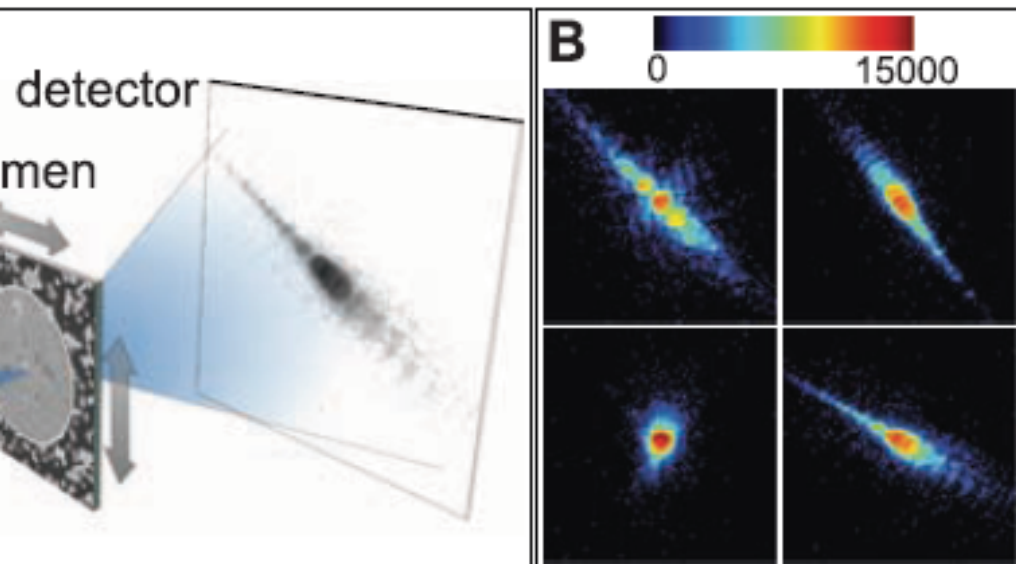
Expansion of the surface layers of a faceted hemispherical nanocrystal of Pb is reported at a temp just below the melting point. Inversion of the coherent x-ray diffraction pattern yields quantitative dimensional maps of the deformation of the crystal from its equilibrium lattice spacing. Most of the sur the crystal has a clear outward displacement, which decays exponentially into the bulk. This is suppre: the (111) facet itself and is stronger on the spherical regions, suggesting that it arises from the orien variation of the underlying surface stress.

DOI: 10.1103/PhysRevB.76.115425

PACS number(s): 61.46.Hk, 62.25.+g, 68.35.Gy, †







# High-Resolution Scanning X-ray Diffraction Microscopy

Pierre Thibault,<sup>1\*</sup> Martin Dierolf,<sup>1</sup> Andreas Menzel,<sup>1</sup> Oliver Bunk,<sup>1</sup> Christian David

Coherent diffractive imaging (CDI) and scanning transmission x-ray microscopy (STXM) are popular microscopy techniques that have evolved quite independently. CDI provides resolutions below 10 nanometers, but the reconstruction procedures put stringent demands on data quality and sample preparation. In contrast, STXM features straightforward reconstruction, but its resolution is limited by the spot size on the specimen. We demonstrate a ptychographic method that bridges the gap between CDI and STXM by measuring complete diffraction patterns at each point of a STXM scan. The high penetration power of x-rays in combination with high spatial resolution will allow investigation of a wide range of complex meso- and nano-scale material science specimens, such as embedded semiconductor devices or cellular

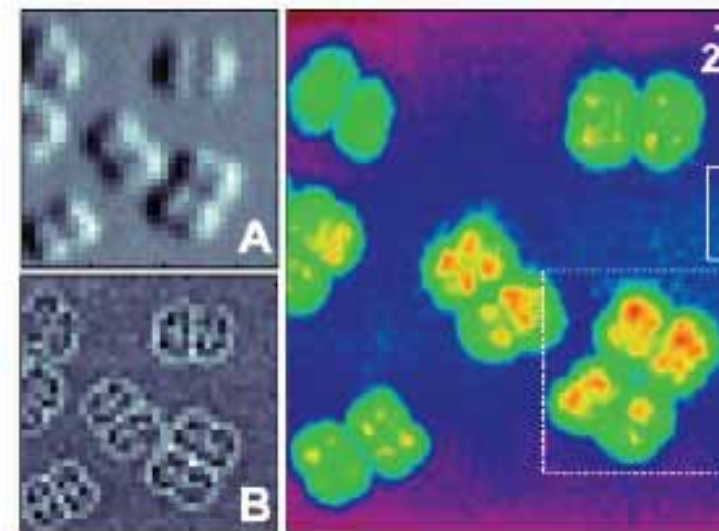
SCIENCE VOL 321 18 JULY 2008

...m past the specimen, thereby removing the need

## Quantitative biological imaging by ptychographic diffraction microscopy

...er<sup>a,1</sup>, Pierre Thibault<sup>b</sup>, Sebastian Kalbfleisch<sup>a</sup>, André Beerlink<sup>a</sup>, Cameron M. Kewish<sup>c</sup>, Martin Dierolf<sup>b</sup>, and Tim Salditt<sup>a,1</sup>

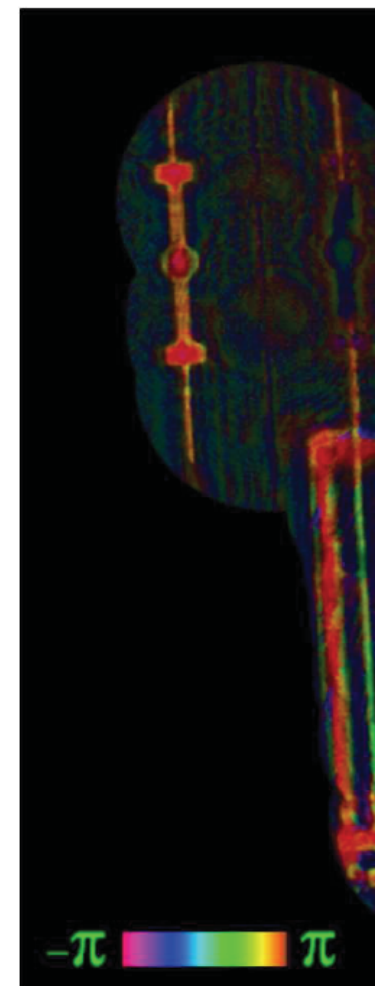
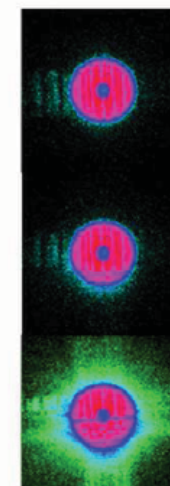
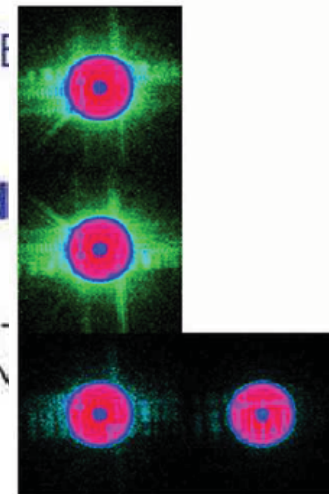
<sup>a</sup>Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany; <sup>b</sup>Department Physik (E17), Universität München, James-Frank-Straße, 85748 Garching, Germany; and <sup>c</sup>Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

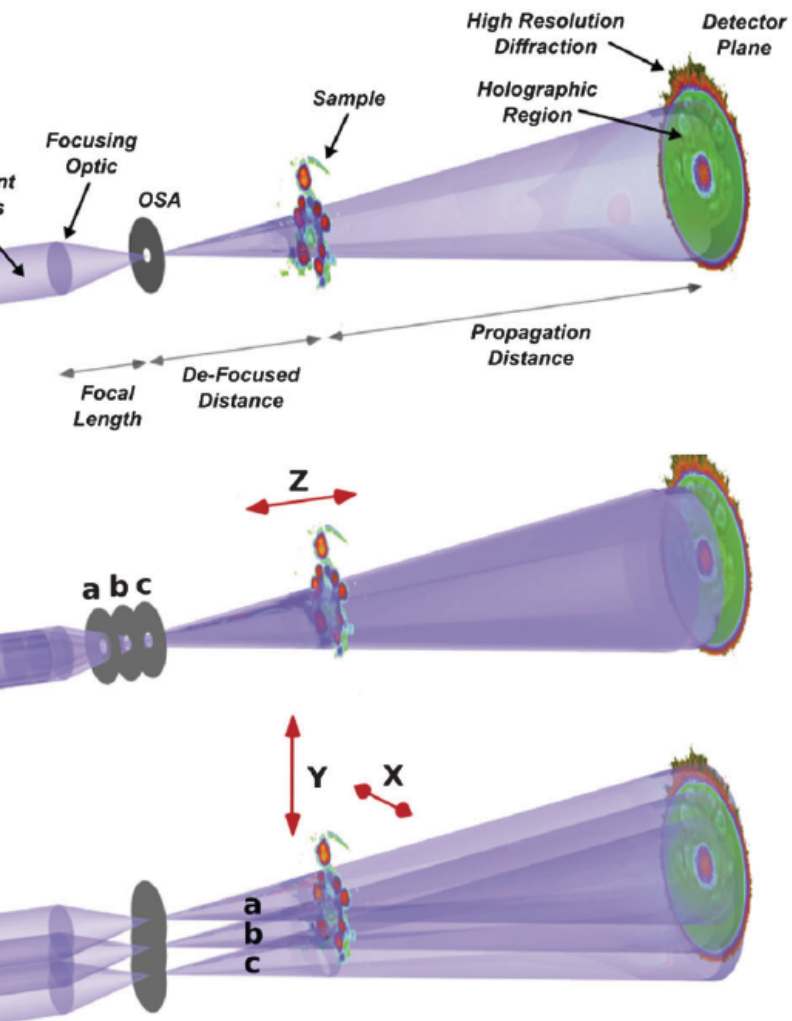


**Fig. 2.** Ptychographic diffractive imaging of freeze-dried cells (1-s dwell time). (A) Differential phase contrast image of the scanned region. One pixel corresponds to one scan area ( $400 \times 400 \text{ nm}^2$ ). (B) Dark-field contrast image of the same region as in A. (C) PCDI reconstruction of the object transmission for the same region as shown in A and B. The area marked by the dashed white frame was scanned again in a subsequent scan with long dwell time.

**Fresnel Coherent Diffractive Imaging**I. Quiney,<sup>1</sup> B. B. Dhal,<sup>1</sup> C. Q. Tran,<sup>1</sup> K. A. Nugent,<sup>1</sup> A. G. Peele,<sup>2</sup> D. Paterson,<sup>3,\*</sup> and M. D. de Jonge<sup>3</sup>**LETTERS**

## Fresnel coherent diffractive imaging

G. J. WILLIAMS<sup>1</sup>, G. J. WILLIAMS<sup>1\*</sup>, JESSE N. CLARK<sup>2</sup>, ANDREW G. PEELE<sup>2</sup>  
APPLIED PHYSICS LETTERS **93**, 214101 (2008)**Fresnel coherent diffractive imaging of an integrated circuit with a resolution of 20 nm**C. ABBEY,<sup>1,a)</sup> Garth J. Williams,<sup>1,a)</sup> Mark A. Pfeifer,<sup>2</sup> Jesse N. Clark,<sup>2</sup> Corey M. S. Torrance,<sup>1</sup> Ian McNulty,<sup>3</sup> T. M. Levin,<sup>4</sup> Andrew G. Peele,<sup>2</sup> and Keith A. Nugent<sup>1</sup>



# Phase retrieval with transverse translation diversity: a nonlinear optimization approach

Manuel Guizar-Sicairos and James R. Fienup

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[mguizar@optics.rochester.edu](mailto:mguizar@optics.rochester.edu), [fienup@optics.rochester.edu](mailto:fienup@optics.rochester.edu)

011) PHYSICAL REVIEW LETTERS

week ending  
7 JANUARY 2011

## Diverse Coherent Diffractive Imaging: High Sensitivity with Low Dose

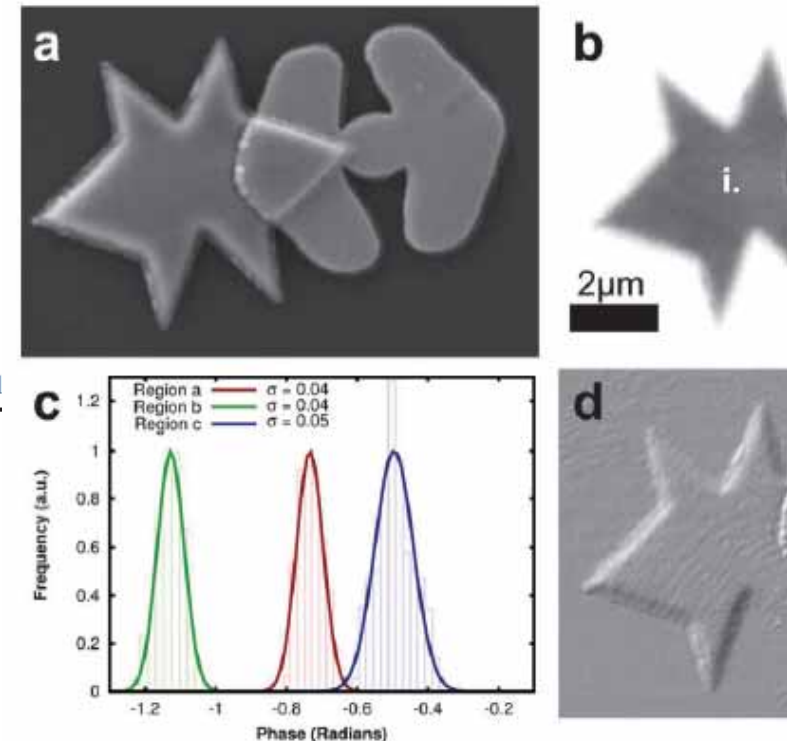
<sup>1,3</sup> Jesse N. Clark,<sup>1,3</sup> David J. Vine,<sup>2,3</sup> Garth J. Williams,<sup>2,3</sup> Mark A. Pfeifer,<sup>1,3</sup> Eugeniu Balaur,<sup>1,3</sup> Ian McNulty,<sup>4</sup> Keith A. Nugent,<sup>2,3</sup> and Andrew G. Peele<sup>1,3,\*</sup>

<sup>1</sup>Department of Physics, La Trobe University, Victoria 3086, Australia

<sup>2</sup>School of Physics The University of Melbourne, Victoria 3010, Australia

<sup>3</sup>Australian Research Council Centre of Excellence for Coherent X-Ray Science

<sup>4</sup>Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA



■  

---

  
Over the past decade, Coherent Imaging has been modified by:

extending the method to 3D imaging

utilizing the intensity around Bragg peaks

using a “curved wavefront”

developing a scanning geometry

introducing “diversity” in the experiment and utilizing

presence in the reconstruction

one of which deals with the source of x-rays!

---

late, neither third- nor fourth-generation sources produce radiation that meets the stringent requirements of CDI:

Storage rings (insertion devices) produce illumination with very many coherent modes

FEL light still has several coherent modes

we exploit explicitly the coherence properties of a source, to what limits and to what advantage?

Can we exploit known coherence properties?

Yes! This propagation of such light is understood

What can we gain?

Less beam conditioning

Shorter exposure times

What's the catch?

The detailed properties of the light must be understood

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Nugent

Quiney

Vine

Abbey

en

Cadenazzi

n Whitehead

Henderson

## **LaTrobe University**

Andrew Peele

Eugeniu Balaur

Jesse Clark

Corey Putkunz

## **Australian Synchrotron**

David Paterson

Martin De Jonge

## **Advanced Photon Source**

Ian McNulty

## **Funding**

The US Department of Energy under contracts governing the APS

The Australian Research Council

ANSTO, under the terms of the ASRP

I measures

$$I(\mathbf{s}) \simeq \int \int \exp[-2\pi i \mathbf{s} \cdot (\mathbf{r}_2 - \mathbf{r}_1)] J(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2$$

ere

$$J(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1) \phi^*(\mathbf{r}_2) g(\mathbf{r}_1 - \mathbf{r}_2)$$

he mutual optical intensity depending on two in-plane 2D vectors and

$$g(\mathbf{r}_1 - \mathbf{r}_2) = \exp\left(\frac{-|\mathbf{r}_1 - \mathbf{r}_2|^2}{2\sigma^2}\right)$$

he coherence function.



Following Wolf, the mutual optical intensity can be rewritten:

$$J(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1)\phi^*(\mathbf{r}_2)g(\mathbf{r}_1, \mathbf{r}_2) = \sum_n \lambda_n \psi_n^*(\mathbf{r}_1)\psi_n(\mathbf{r}_2)$$

Each  $\psi_n$  is a “coherent mode.”

⇒ each mode must obey the support constraint

⇒ *we can propagate partially coherent scattering!*

Flewett, et al., Opt. Lett. 34, 2198 (2009)

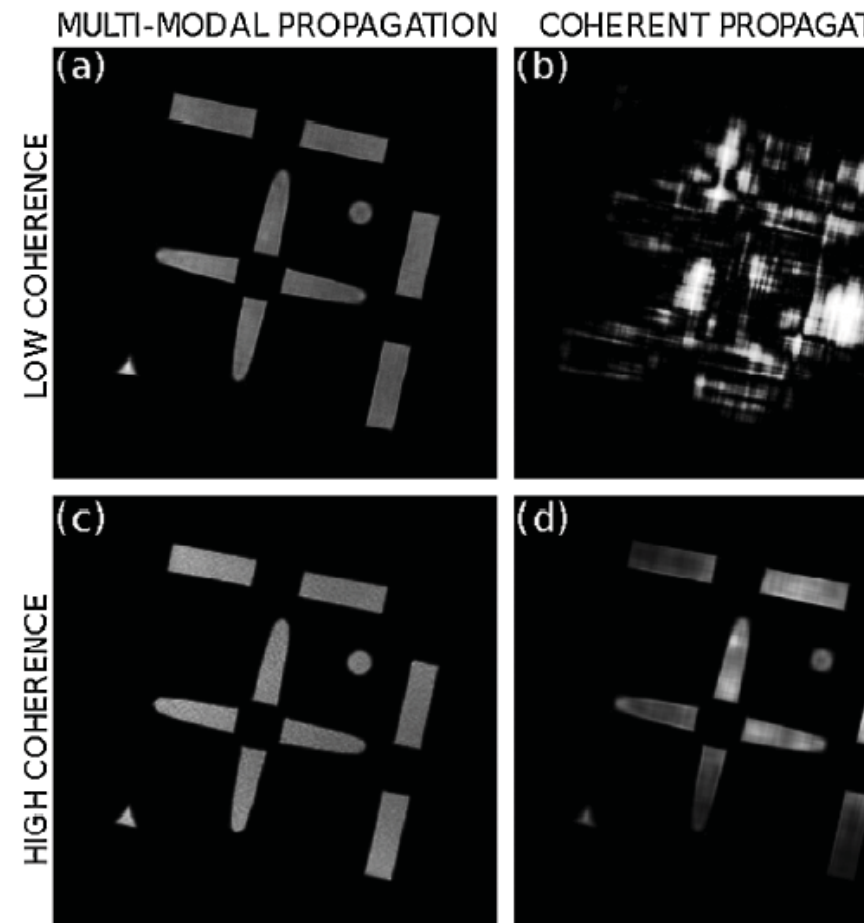
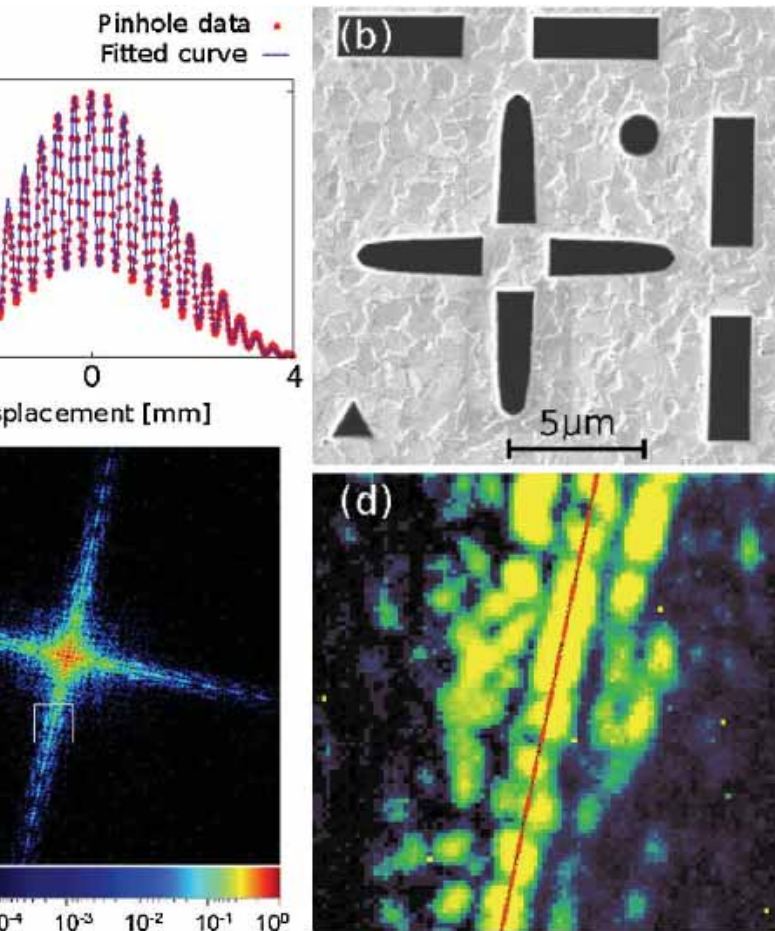
## Diffractive Imaging Using Partially Coherent X Rays

L. W. Whitehead, G. J. Williams, H. M. Quiney, D. J. Vine, R. A. Dilanian, S. Flewett, and K. A. Nugent  
*School of Physics, The University of Melbourne, Victoria 3010, Australia*

A. G. Peele and E. Balaur  
*Department of Physics, La Trobe University, Bundoora, Victoria 3086, Australia*

I. McNulty

*Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois, 60439, USA*  
 (Received 26 August 2009; revised manuscript received 18 November 2009; published 11 December 2009)



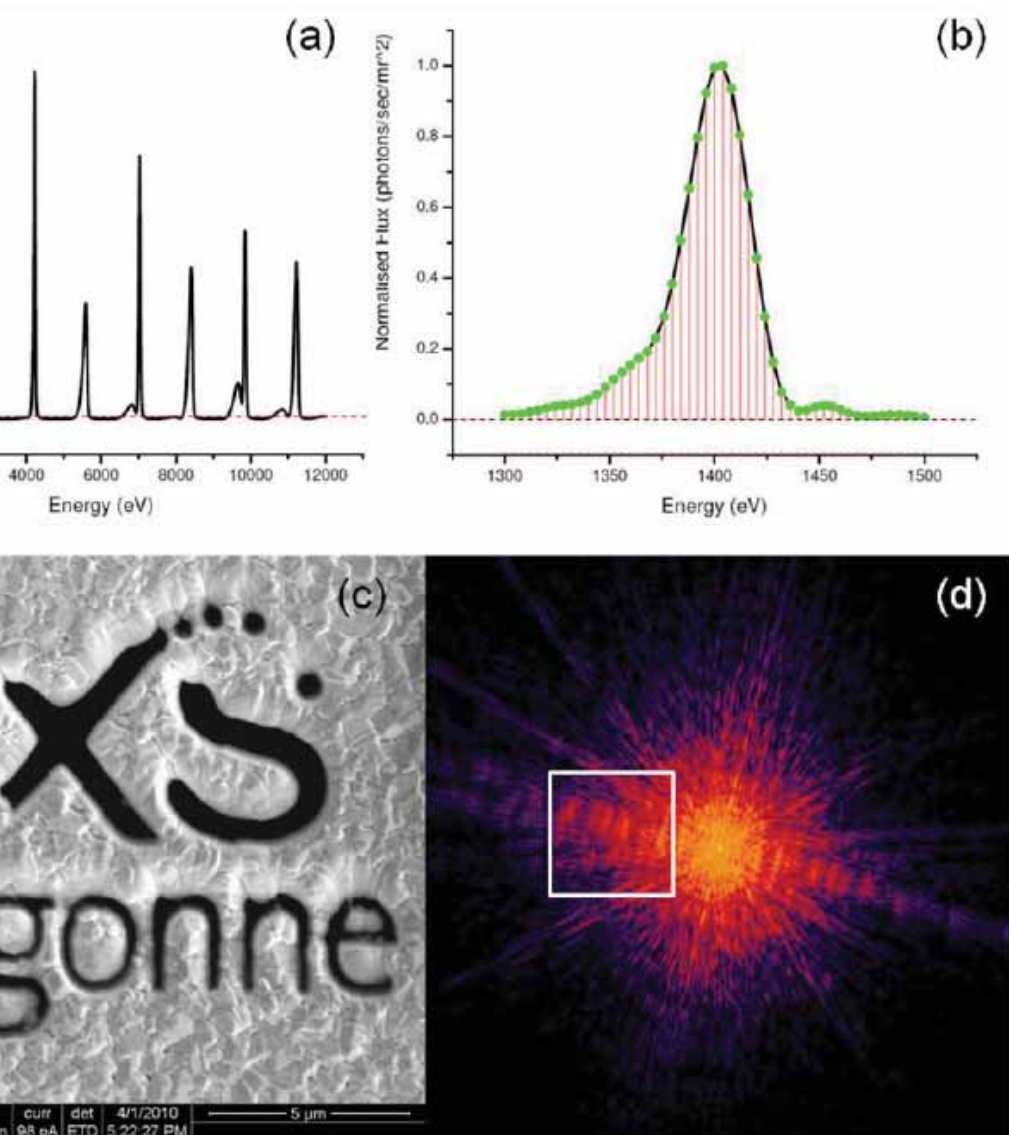
It propagates between two planes according to

$$\psi_\lambda(\mathbf{r}_j, z_j) = -\frac{i}{\lambda z} \exp\left(\frac{2\pi i z_{\bar{v}}}{\lambda}\right) \exp\left(\frac{i\pi \mathbf{r}_j^2}{\lambda z_{\bar{v}}}\right) \iint \psi_\lambda(\mathbf{r}_i, z_i) \exp\left(-\frac{2\pi i \mathbf{r}_i \cdot \mathbf{r}_j}{\lambda z_{\bar{v}}}\right) d\mathbf{r}_i$$

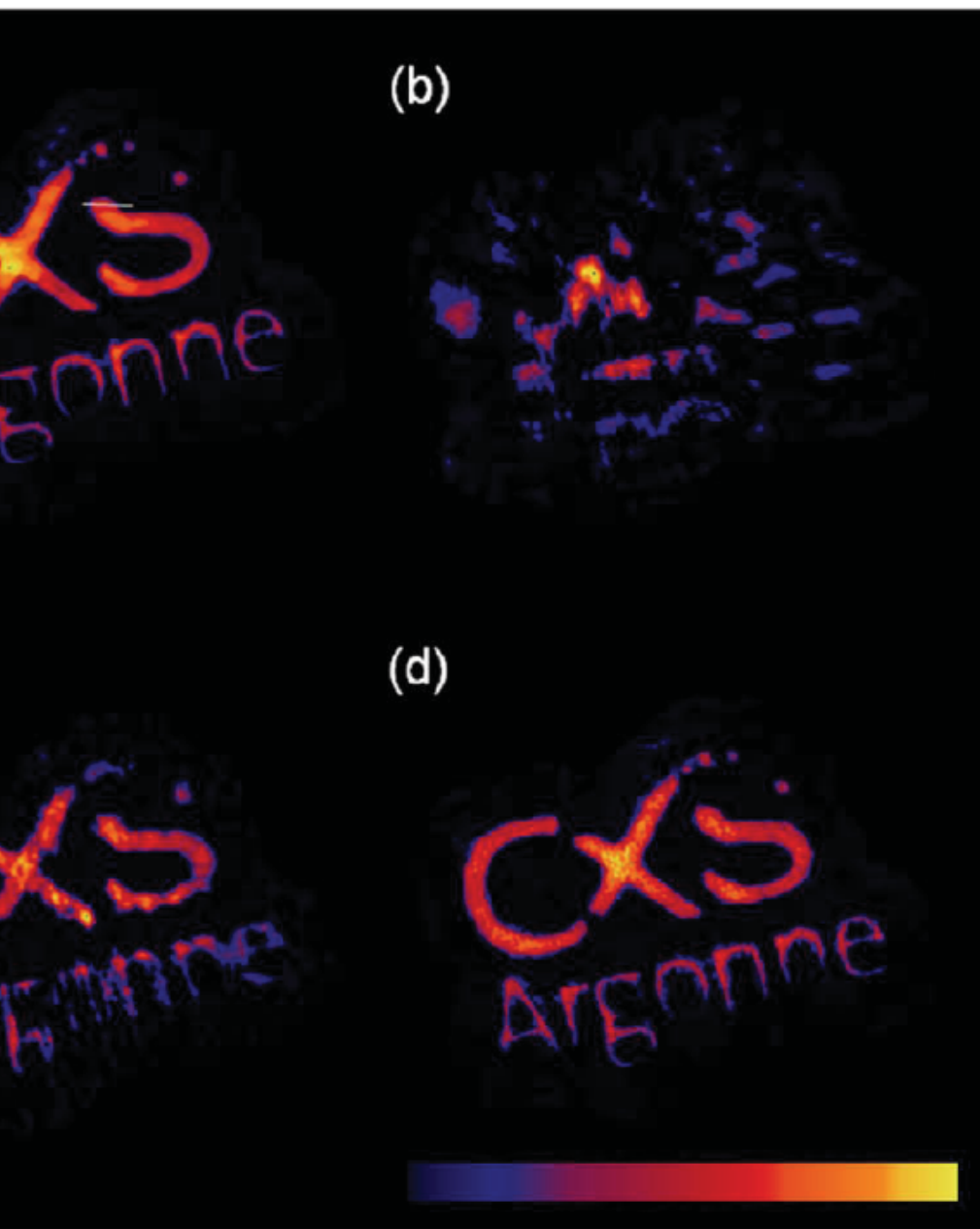
Therefore, the total intensity in the detector plane can be written as

$$I(\mathbf{r}_j, \mathbf{z}_j) = \int \xi_\lambda |\psi_\lambda(\mathbf{r}_j, \mathbf{z}_j)|^2 d\lambda$$

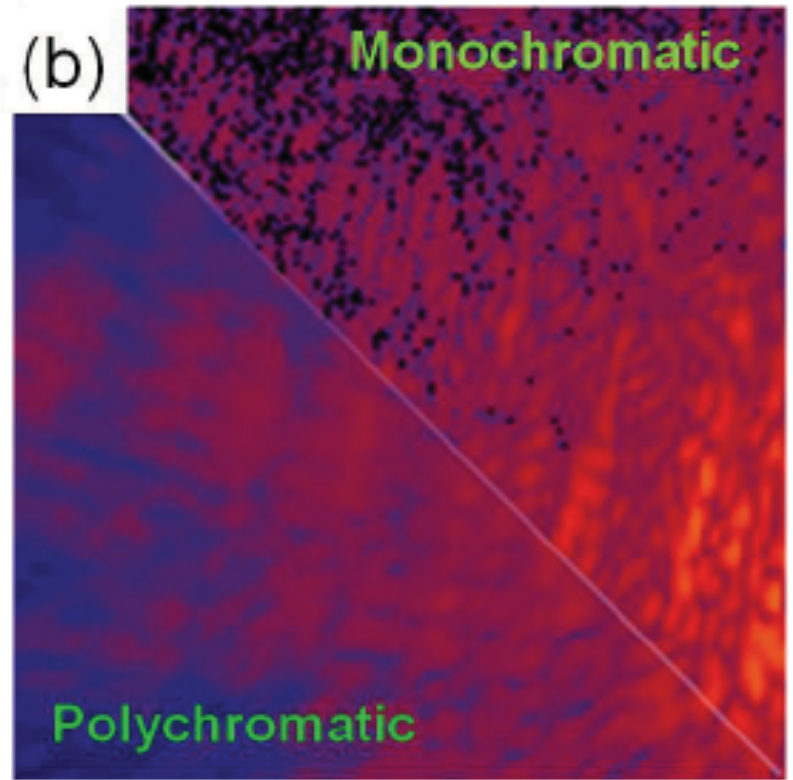
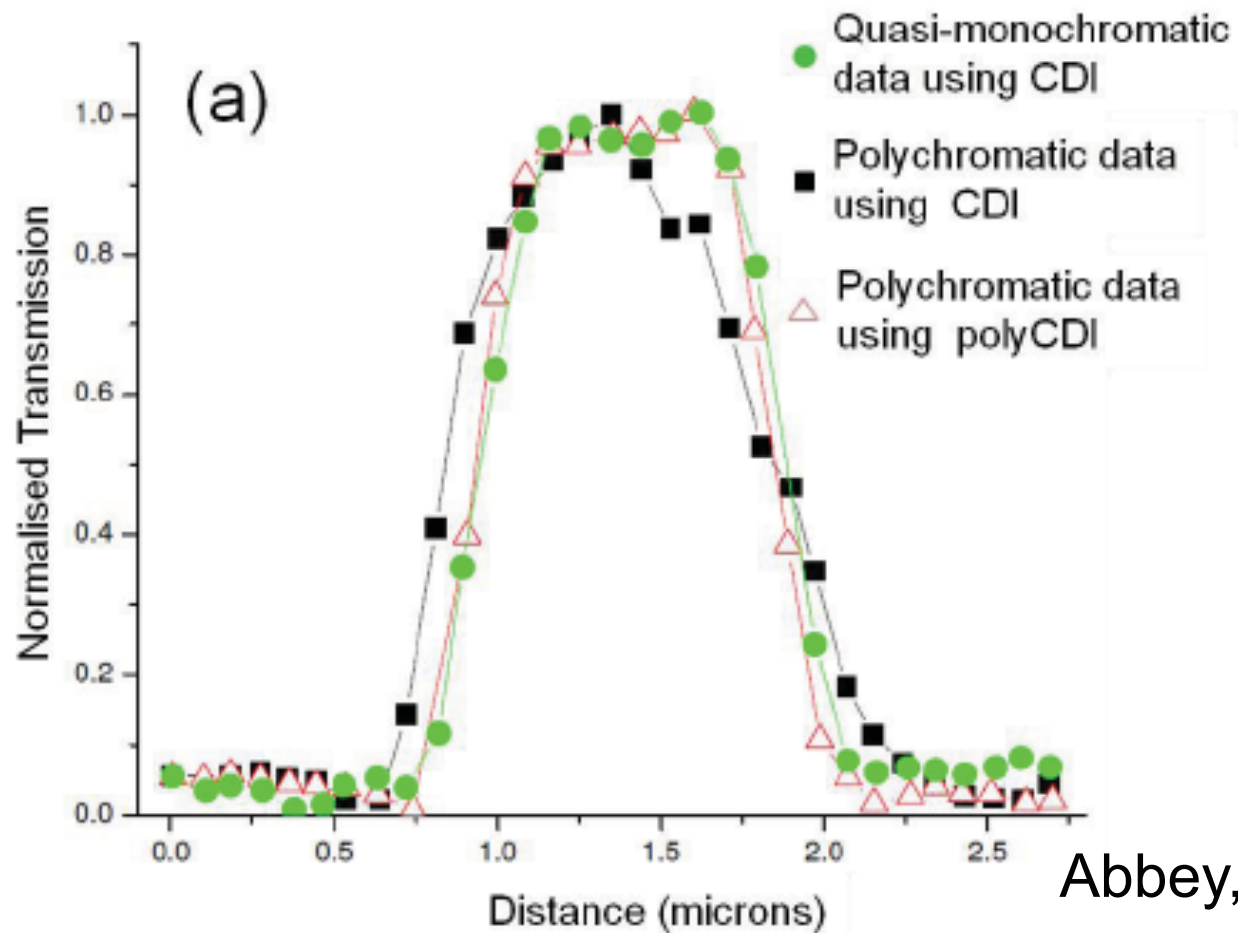
This forms the basis of an algorithmic strategy for broadband illumination CDI!



- The undulator spectrum is discretised
- A test sample is milled from a Au
- A partially coherent diffraction pattern from the sample



- (a) and (d) show that monochromatic and polychromatic CDI are not sufficient to reconstruct the image at the same solution
- Intermediate frames show the consequences of ignoring the partial coherence



Abbey, et al., accepted by Nature Phot

Comparison of reconstruction fidelity (left)

Graphical depiction of the effect of decreased longitudinal coherence on the diffraction from the sample

increases acceptable band-width of illumination from  $\sim 1\%$  to  $\sim 11\%$

in this example, reduces exposure time by factor of 60

transverse coherence can be accommodated at limitations very similar to traditional CI

complicated when the illumination includes resonant edges

---

CDI has made very good progress toward becoming  
an alternative to x-ray microscopy

There exist many examples of the advantages of  
CDI, explicitly including characterized beam properties and  
simple motions, including algorithmic stability and  
extending the method to new samples

The inclusion of the coherence properties of  
synchrotron radiation has many potential benefits including: a  
reduction of the sample exposure time and the  
extension of the method to higher x-ray energies  
A bright, stable source is a huge advantage for CDI



1. An initial guess is made for the sample ESW:  $\psi(\mathbf{r}_i, z_i)$ .
2. The result is propagated to the far-field via (1) to give the central wavelength distribution  $\psi_c(\mathbf{r}_j, z_j)$  and scaled by a factor appropriate to  $\lambda_{\max}$  to yield  $\psi(\mathbf{r}_j, z_j)_{\lambda_{\max}}$ .
3. The positions  $\mathbf{r}_j$  for the other sampled wavelengths are rescaled according to  $\mathbf{r}_j(\lambda_{\max} - \Delta\lambda) / \lambda_{\max}$ .
4. The diffraction patterns from each sampled wavelength are calculated via interpolation onto the new set of points defined by the rescaled values for  $\mathbf{r}_j$ .
5. The intensity distribution from each pattern is multiplied by a weighting factor determined by the relative contribution of each wavelength to the frequency spectrum:

$$\xi_\lambda |\psi_\lambda(\mathbf{r}_j, z_j)|^2.$$

- 
6. The sum of the distributions for each sampling point approximates the integral in eq(4) which gives the calculated polychromatic diffraction pattern:

$$I(\mathbf{r}_j, \mathbf{z}_j) = \int \xi_\lambda |\psi_\lambda(\mathbf{r}_j, \mathbf{z}_j)|^2 d\lambda.$$

7. The modulus constraint is imposed using:  $|\psi_c(\mathbf{r}_j, \mathbf{z}_j)| * \sqrt{I(\mathbf{r}_j, \mathbf{z}_j)_{meas}} / \sqrt{I(\mathbf{r}_j, \mathbf{z}_j)}$

where  $I(\mathbf{r}_j, \mathbf{z}_j)_{meas}$  is the measured intensity from experiment.

8. With the amplitude updated, the phase of  $\psi_c(\mathbf{r}_j, \mathbf{z}_j)$  is retained and the ESW propagated back to the sample plane to give,  $\psi(\mathbf{r}_i, z_i)$ , after which the support constraint is imposed.

9. Steps 1-9 are repeated and the progress of the reconstruction monitored using an error metric defined as:  $\chi^2 = \left( \sqrt{I(\mathbf{r}_j, \mathbf{z}_j)_{meas}} - \sqrt{I(\mathbf{r}_j, \mathbf{z}_j)} \right)^2 / I(\mathbf{r}_j, \mathbf{z}_j)$ .